

Thermophysical Property Sensitivity Effects in Steel Solidification

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The simulation of advanced solidification processes via digital computer techniques has gained widespread acceptance during the last decade or so. Models today can predict transient temperature fields, fluid flow fields, important microstructural parameters, and potential defects in castings. However, the lack of accurate thermophysical property data on important industrial alloys threatens to limit the ability of manufacturers to fully capitalize on the technology's benefits. This paper describes a study of the sensitivity of one such numerical model of a steel plate casting to imposed variations in the data utilized for the thermal conductivity, specific heat, density, and heat of fusion. The sensitivity of the data's variability is characterized by its effects on the net solidification time of various points along the centerline of the plate casting. Recommendations for property measurements are given and the implications of data uncertainty for modelers are discussed.

Simulation results can only be as good as the boundary conditions/heat transfer coefficients applied and the thermophysical properties used, i.e., density, specific heat, latent heat, and thermal conductivity. Several other authors have investigated the important effects of interfacial heat transfer coefficients and found a strong dependency of the evolution of the thermal field on these coefficients. However, few modelers cite more than a passing concern for the lack of thermophysical data and the uncertainty inherent in the data that is available. Depending on the source of thermophysical property data, considerable errors may be present. For example, the data for the thermal conductivity of tungsten reported in the literature exhibits as much as 300% scatter even though many data sets are reported to be accurate to within 1% or less! In addition, the data for a great many complex alloys of industrial interest are simply unavailable.

The casting chosen for this study is the solidification of a horizontal steel plate in green sand with a riser at one end as shown in Figure 1. This is the same geometry investigated by Minakawa *et al*¹ in their study of the feeding of porosity. The nominal properties used were identical to those of Minakawa *et al* and are shown in Table I. The thickness of the plate is 25 mm and the length is 200 mm. Centerline shrinkage has been observed to occur in the region indicated in Figure 1.² The assumptions made by Minakawa *et al* were repeated here. (1) The mold is instantaneously filled with molten metal at the pouring temperature. (2) The thermal contact resistance at the metal-sand mold interface is negligible. (3) Segregation is neglected. (4) The latent heat is released uniformly between the liquidus temperature and the solidus temperature irrespective of cooling rate effects.

The model was tested by comparing calculations of the plate centerline temperatures with the measured temperatures of Bishop and Pellini.² Excellent agreement was found in the temperature range between the solidus and the liquidus.

The effects of various uncertainties upon the predicted solidification times due to uncertainties in the steel's thermal conductivity, specific heat, latent heat and density are shown in Figures 2, 3, 4, and 5 respectively. A comparison of these effects is presented in Figure 6 where the solidification times of the node at 57.1 mm from the plate edge are shown. Increasing the thermal conductivity value of the steel by 100% only decreased the time to solidify by about 13%. An error of +50% in the specific heat of the steel would cause an increase in the predicted time to freeze of ~25%, whereas a

+50% error in the latent heat would increase the predicted solidification time by 55%. The sensitivity of the model is even greater to variations in the density used. The predicted solidification time increased by 90% with a +50% error in the steel's density.

In terms of the molten steel's properties, the model investigated was most sensitive to uncertainties in the steel's density and least sensitive to its thermal conductivity. The approximate sensitivity coefficients are:

$$\begin{aligned} \frac{\partial T_f}{\partial K} &= 0.084 \frac{\text{min}}{\text{W/m}^{\circ}\text{K}}, & \frac{\partial T_f}{\partial L_f} &= 5.2 \times 10^{-5} \frac{\text{min}}{\text{J/kg}}, \\ \frac{\partial T_f}{\partial c_p} &= 8.76 \times 10^3 \frac{\text{min}}{\text{J/kg}^{\circ}\text{K}}, & \text{and } \frac{\partial T_f}{\partial \rho} &= 2.88 \times 10^{-3} \frac{\text{min}}{\text{kg/m}^3}. \end{aligned}$$

Although high temperature molten alloys are experimentally difficult, many techniques exist for determining most of these properties required to accuracies of the order of $\pm 5\%$ or better. However, there is little agreement on standard techniques, little publicly available data on most common industrial alloys, and apparently little incentive for researchers to worry about the absolute validity of the data they use. Inaccurate data leads to inaccurate results and can stop a development program in its tracks. All investigators should strive to critically assess the amount of uncertainty in the data that they use and to quantify the expected effects of that uncertainty in their results. The maturation of computer modeling from a research tool to a design tool demands no less.

Conclusions

1. The sensitivity of computer solidification models to uncertainties in thermophysical properties can be readily assessed by straightforward variation of their values in a one-at-a-time manner.
2. Large errors in some of the input thermophysical properties can lead to corresponding large errors in computer models' predictions.
3. For variations up to $\pm 25\%$ in the thermophysical properties, the relative importance of the input properties is: $\text{density}_{\text{steel}} > \text{latent heat}_{\text{steel}} > \text{specific heat}_{\text{steel}} > \text{thermal conductivity}_{\text{steel}}$.

Acknowledgements

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References

1. S. Minakawa, I.V. Samarasekera, and F. Weinberg, "Centerline Porosity in Plate Castings," *Metall. Trans. B*, 16B(1985) pp. 823-829.
2. H.F. Bishop and W.S. Pellini, "The Contribution of Riser and Chill-Edge Effects to Soundness of Cast Steel Plates," *AFS Trans.*, 58(1950) pp. 185-197.

Figure 1

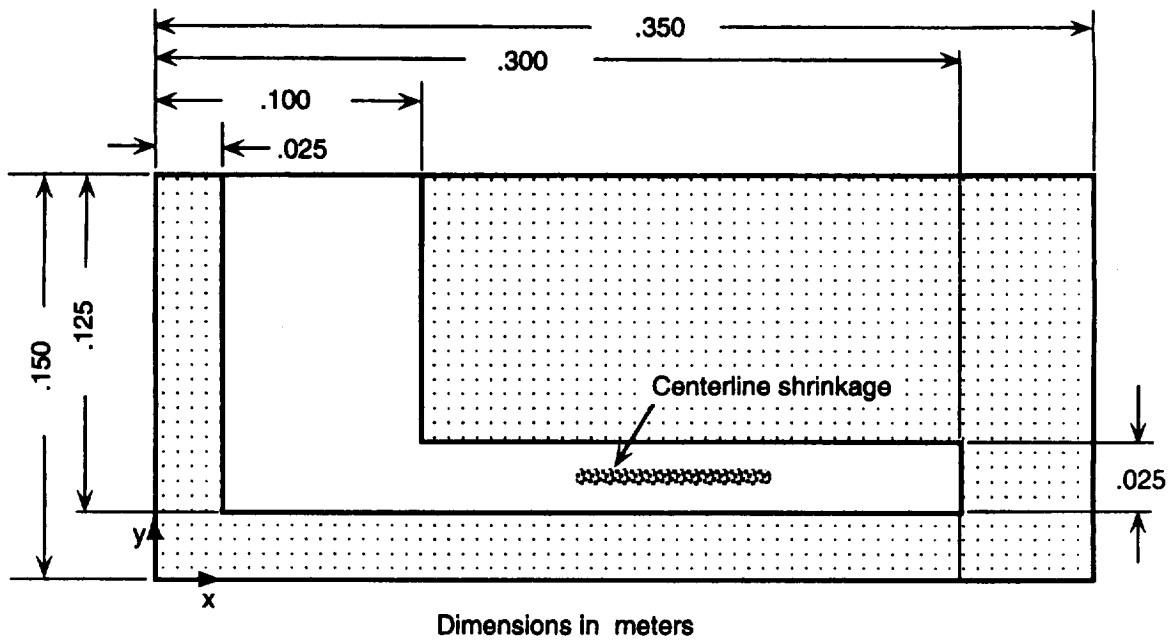


Figure 2
Effects of Uncertainty in Thermal Conductivity

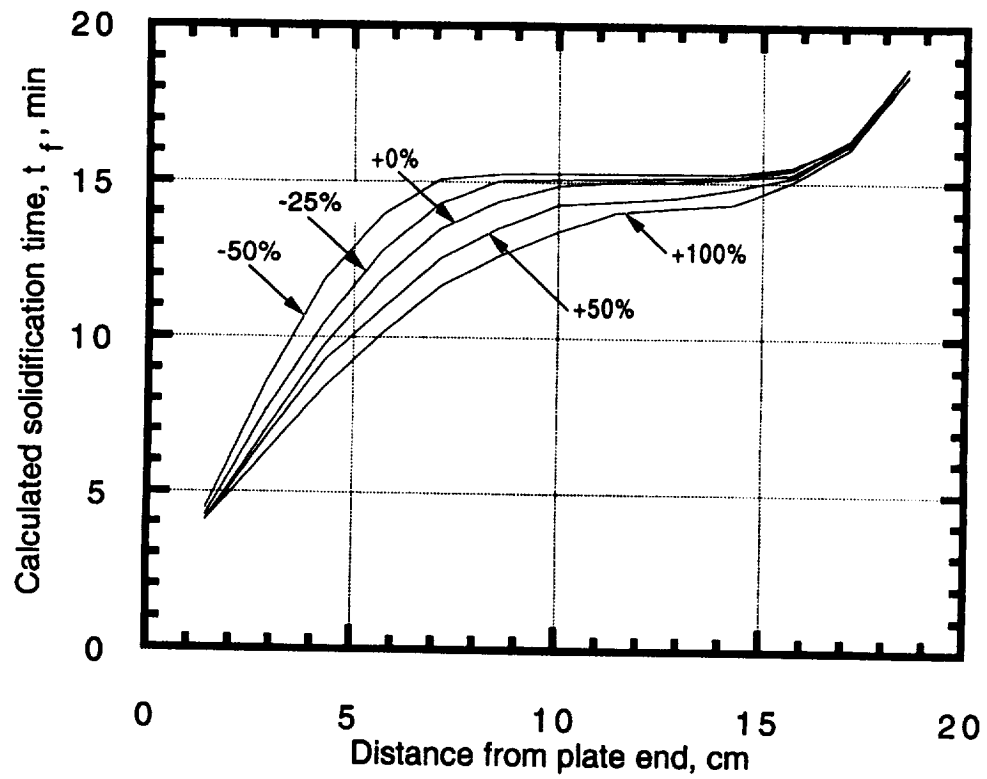


Figure 3
Effects of Uncertainty in Specific Heat

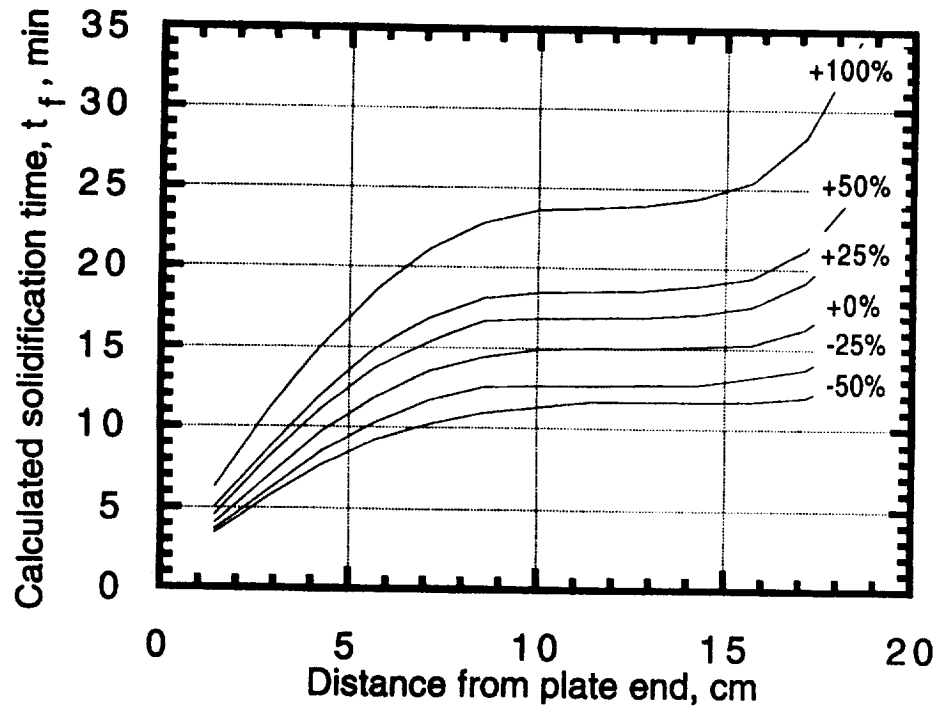


Figure 4
Effects of Uncertainty in Latent Heat

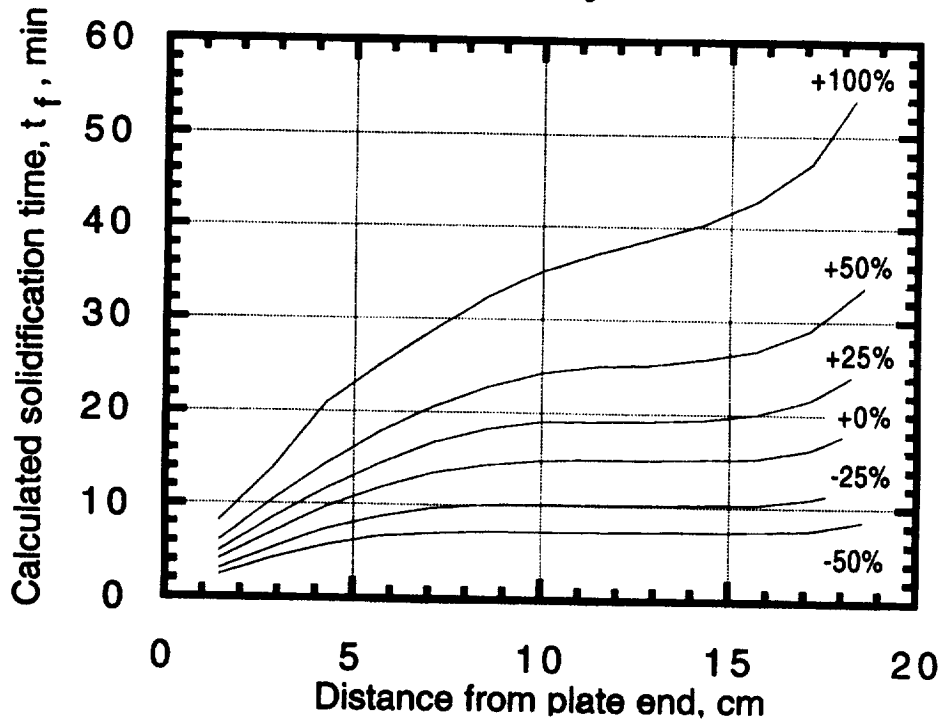


Figure 5
Effects of Uncertainty in Density

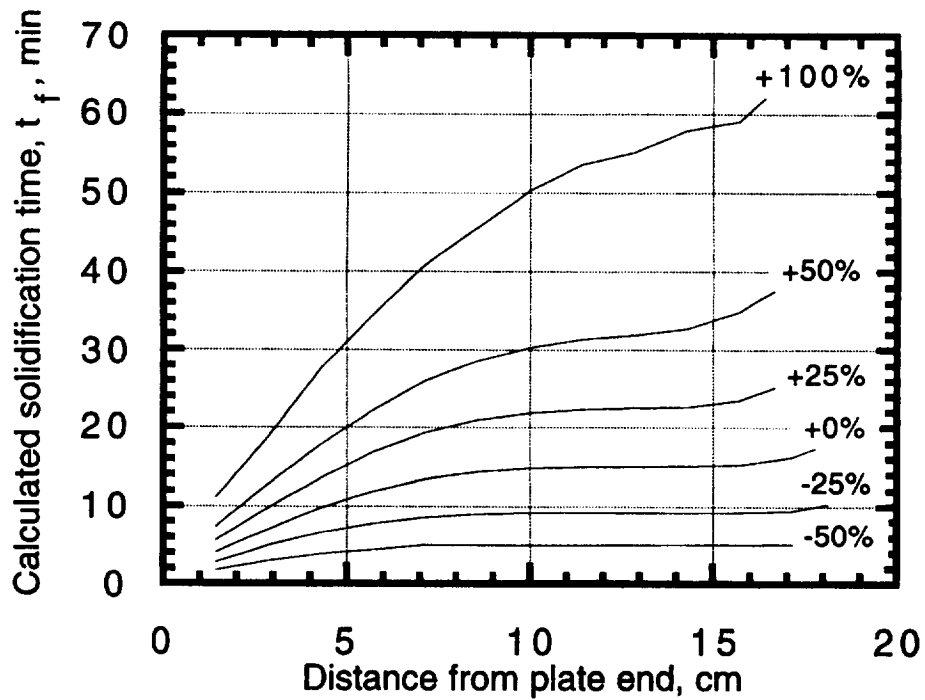
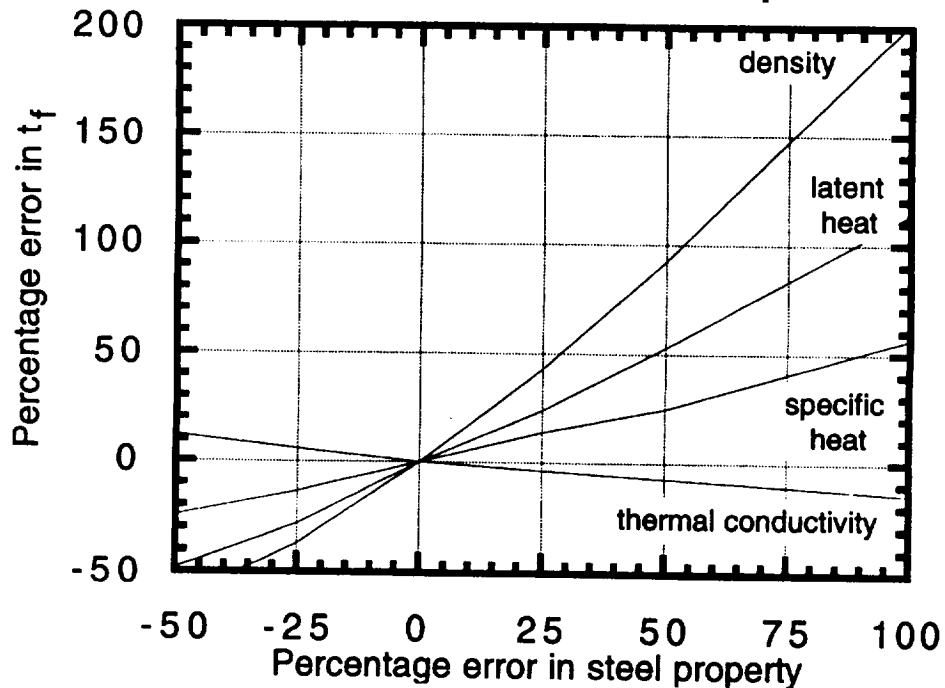


Figure 6
Effects of Errors in Steel Properties



Heat conduction is governed by the following well known unsteady equation:

$$\frac{\partial T}{\partial t} = \frac{K}{\rho c_p} \nabla^2 T + \frac{L_f}{\rho c_p}$$

where T is the temperature

ρ is the density

c_p is specific heat

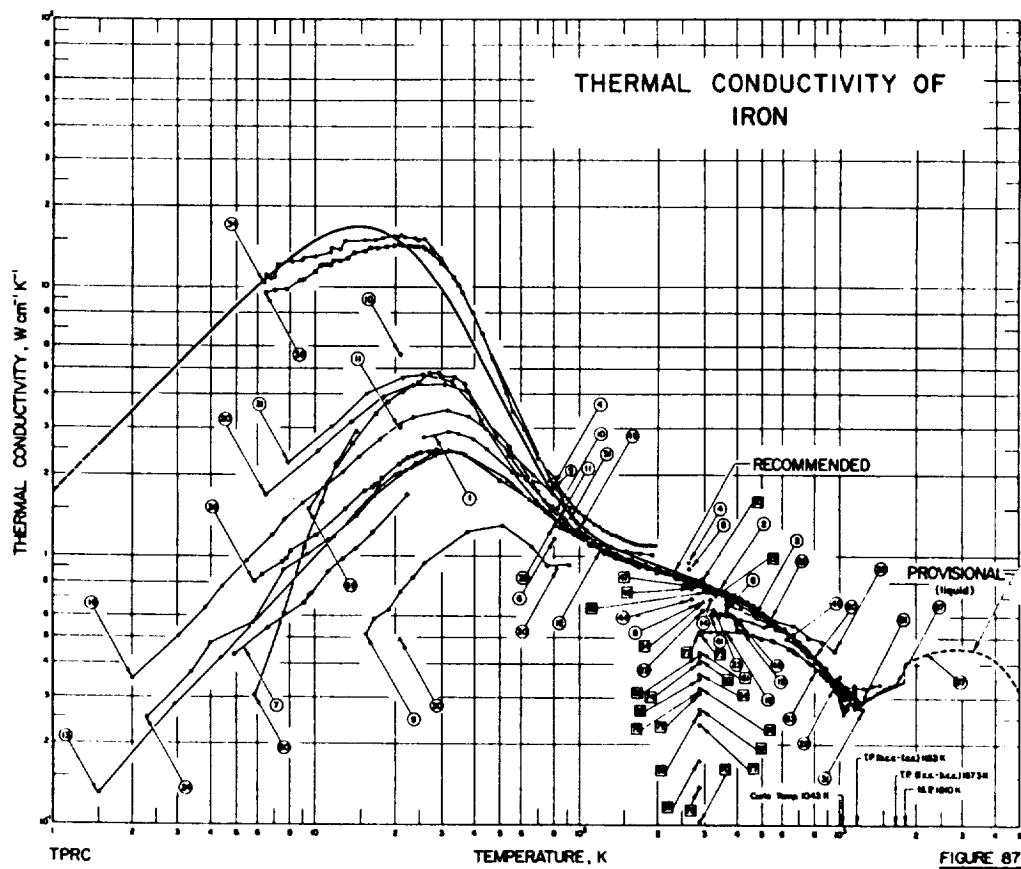
L_f is the latent heat

t is time,

K is the thermal conductivity, and

the properties are independent of temp.

A simple-minded, one-at-a-time variation of the properties in a validated model would quickly give valuable insight into which thermophysical properties are the dominant ones governing heat flow in casting.



C.Y Ho, R.W. Powell, and P.E. Liley, Thermal Conductivity of the Elements: A Comprehensive Review, J. Phys. Chem. Ref. Data, Vol. 3, Supp. No. 1, American Chemical Society and American Institute of Physics, 1974, pp. 1-369.

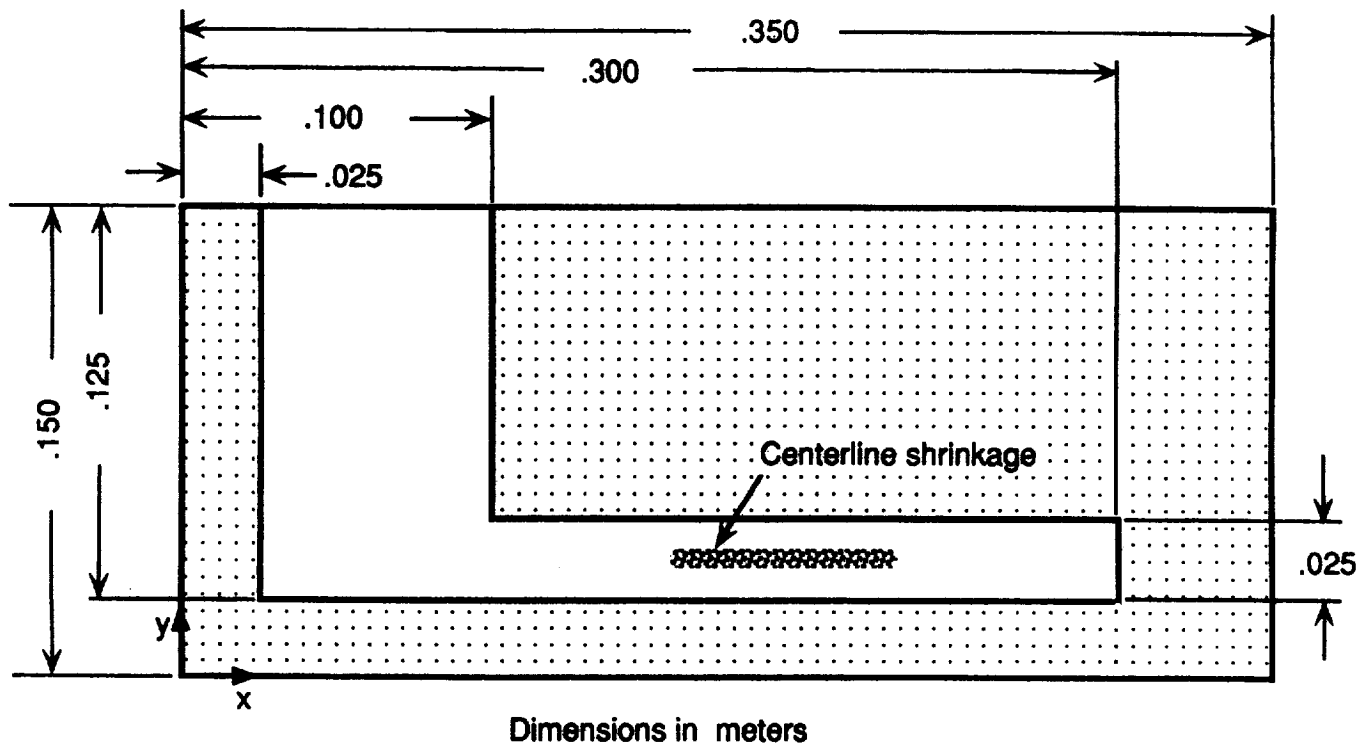
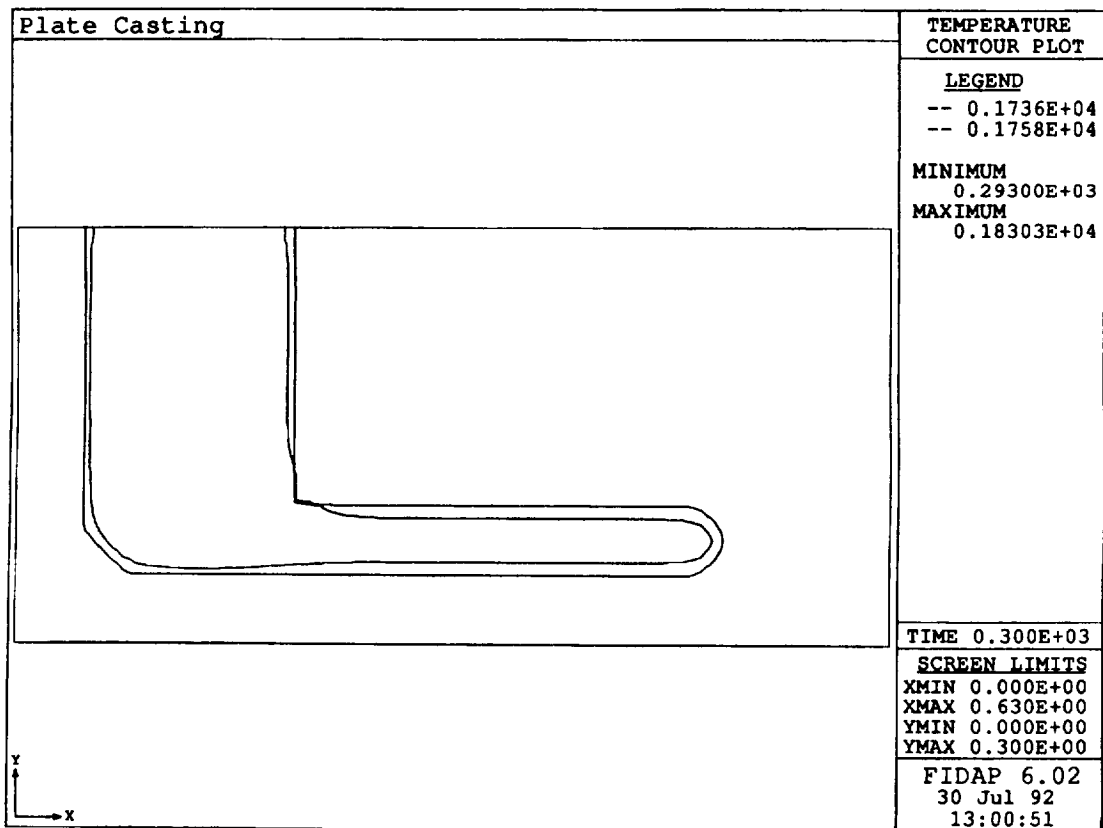
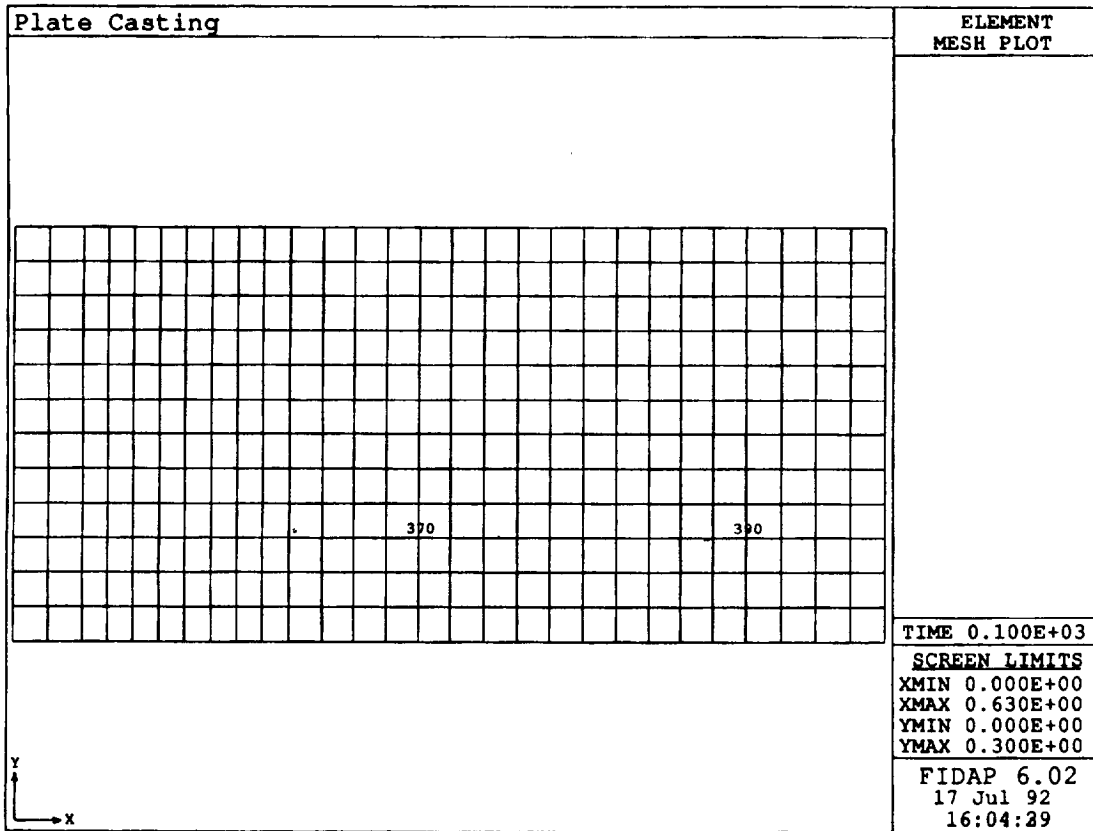
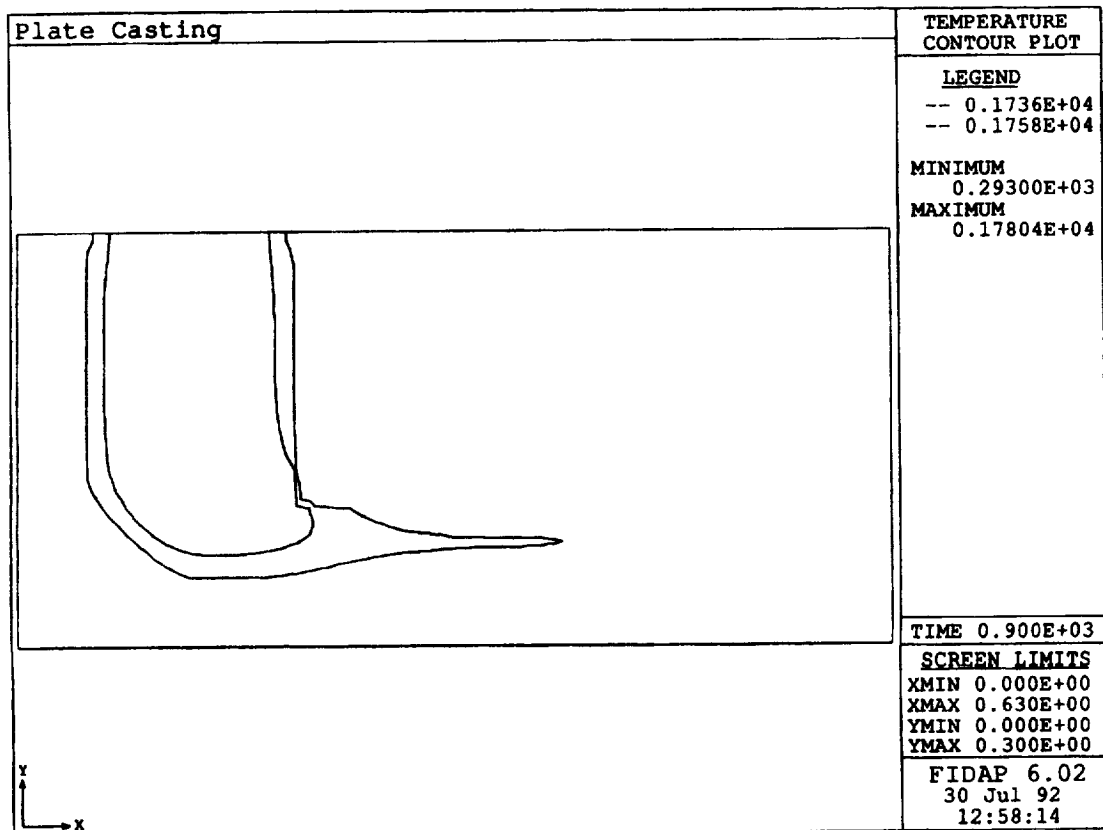
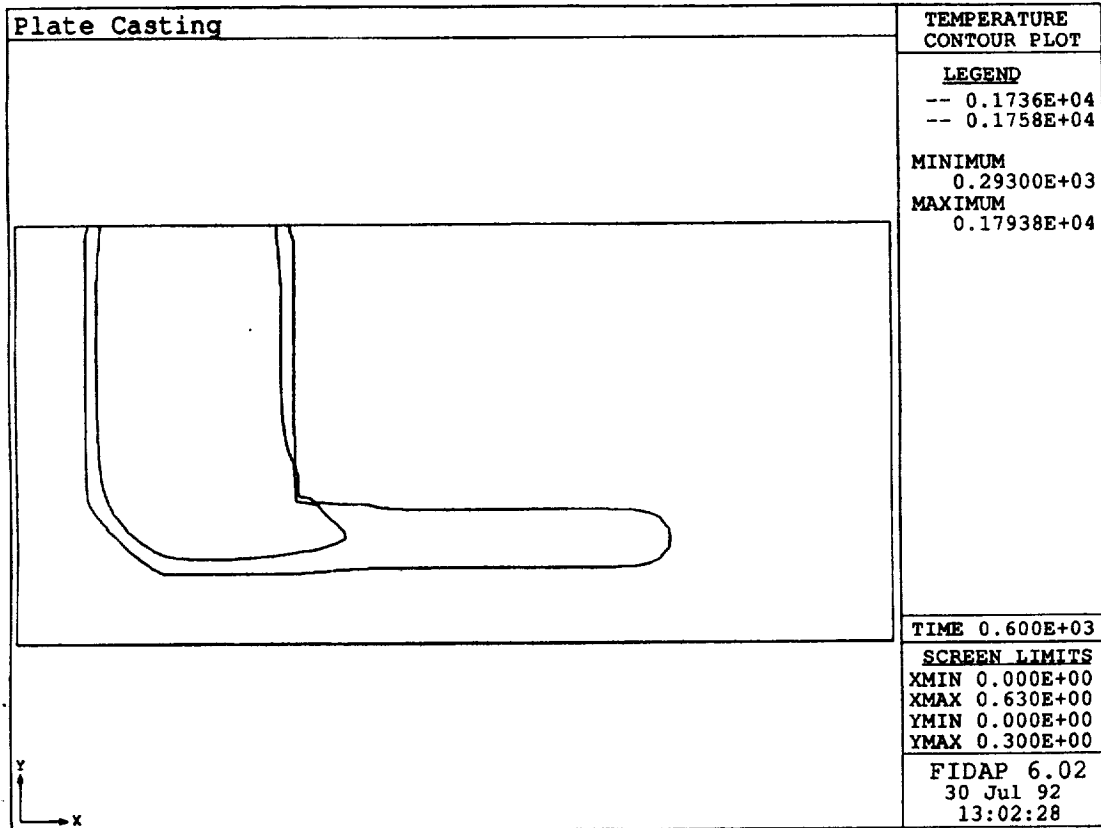


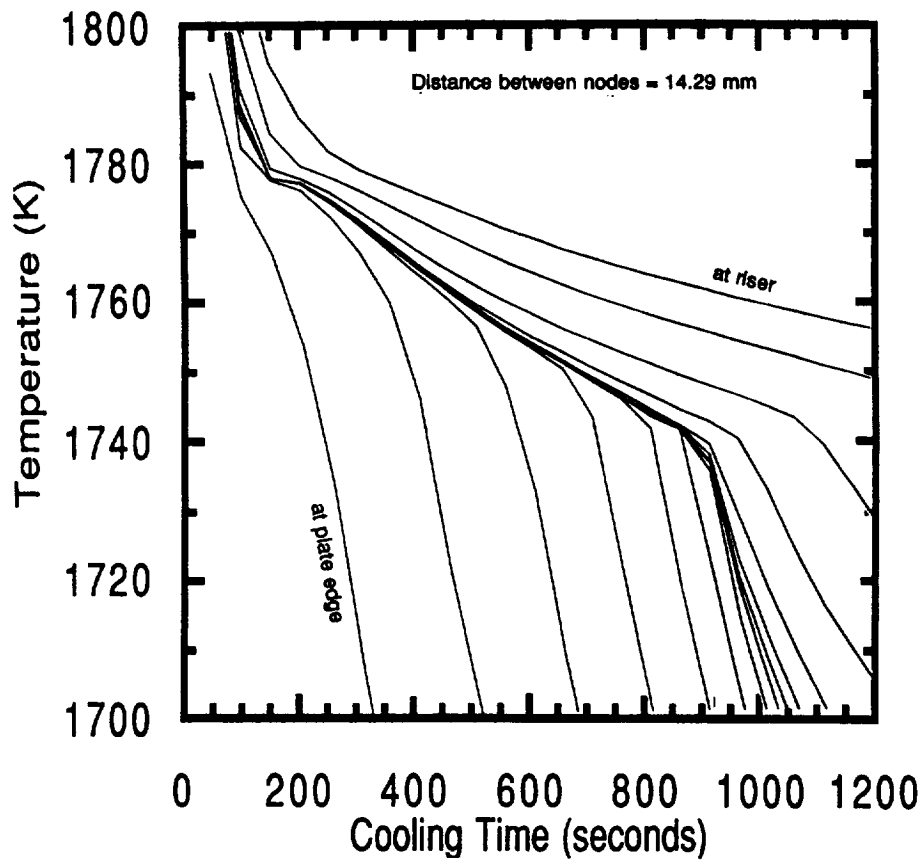
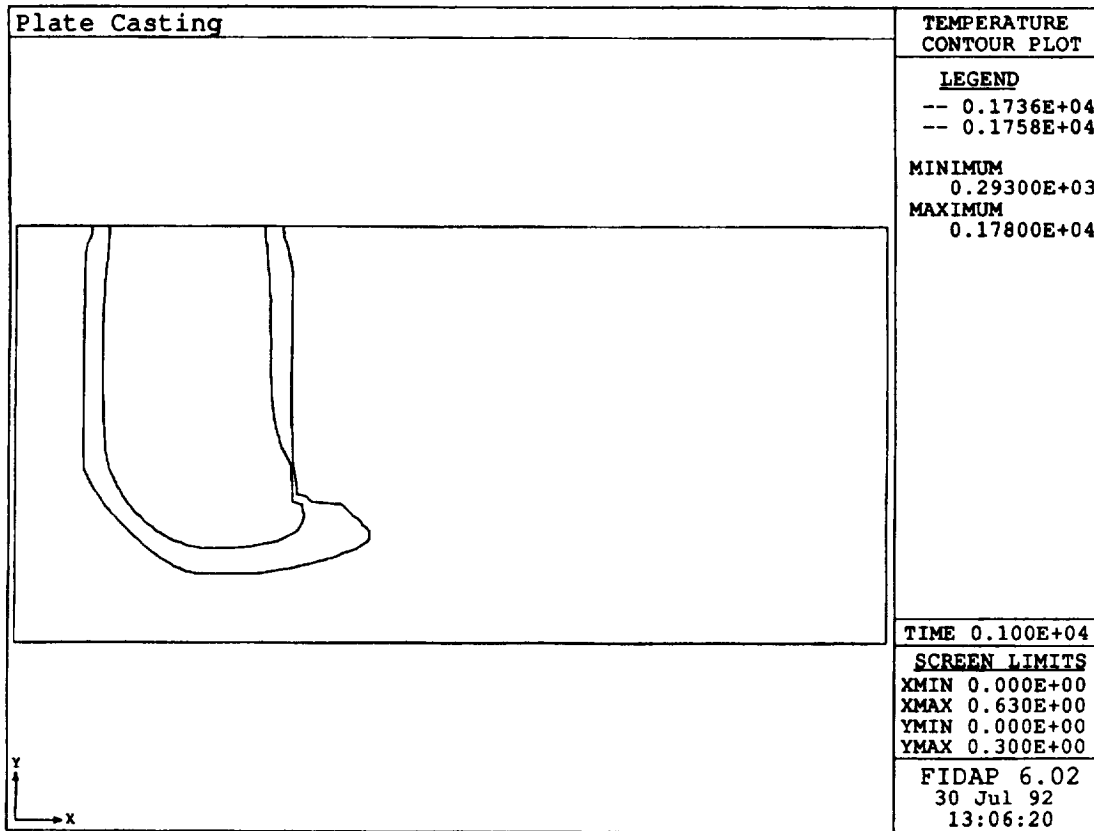
Table I
Nominal Values of the
Physical Data Used in the Calculations

Property or Parameter	Units	Steel	Mold
Specific heat, c_p	J/kg °K	840	1050
Density of liquid, ρ	kg/m ³	7100	
Density of solid, ρ	kg/m ³	7500	1650
Thermal conductivity, k	W/m °K	31	1.55
Heat transfer coefficient, H_s	W/m ² °K		20.9
Latent heat, L_f	J/kg	2.7×10^5	
Liquidus temperature, T_L	°K	1780	
Solidus temperature, T_s	°K	1736	
Pouring temperature, T_p	°K	1868	
Emissivity, ϵ	-	0.45	

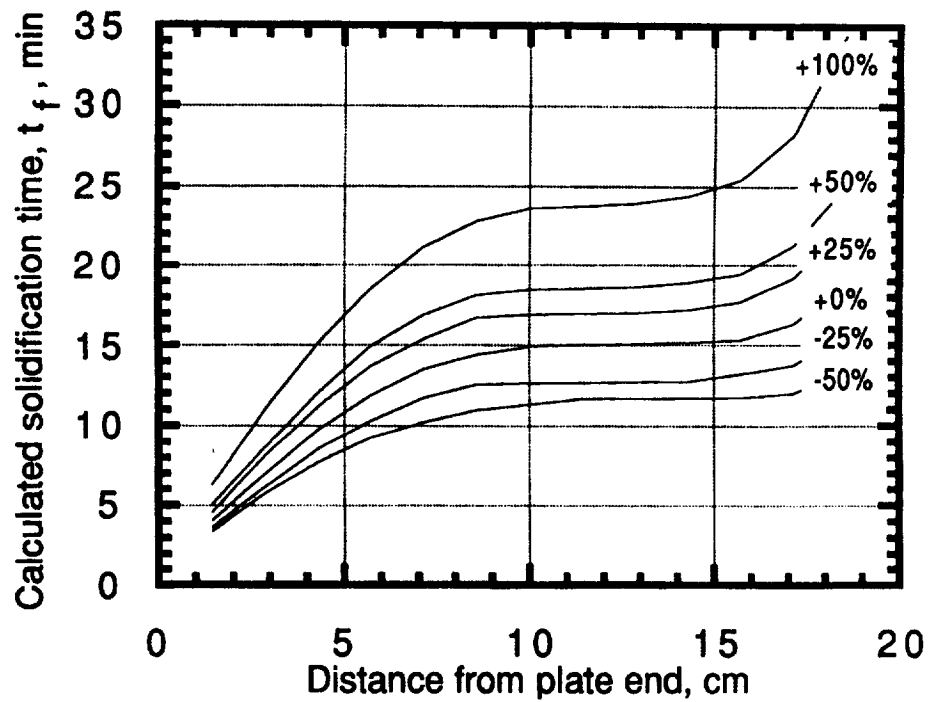
S. Minakawa, I.V. Samarasekera, and F. Weinberg, Metall. Trans. B.
1985, vol. 16B, pp. 823-829.



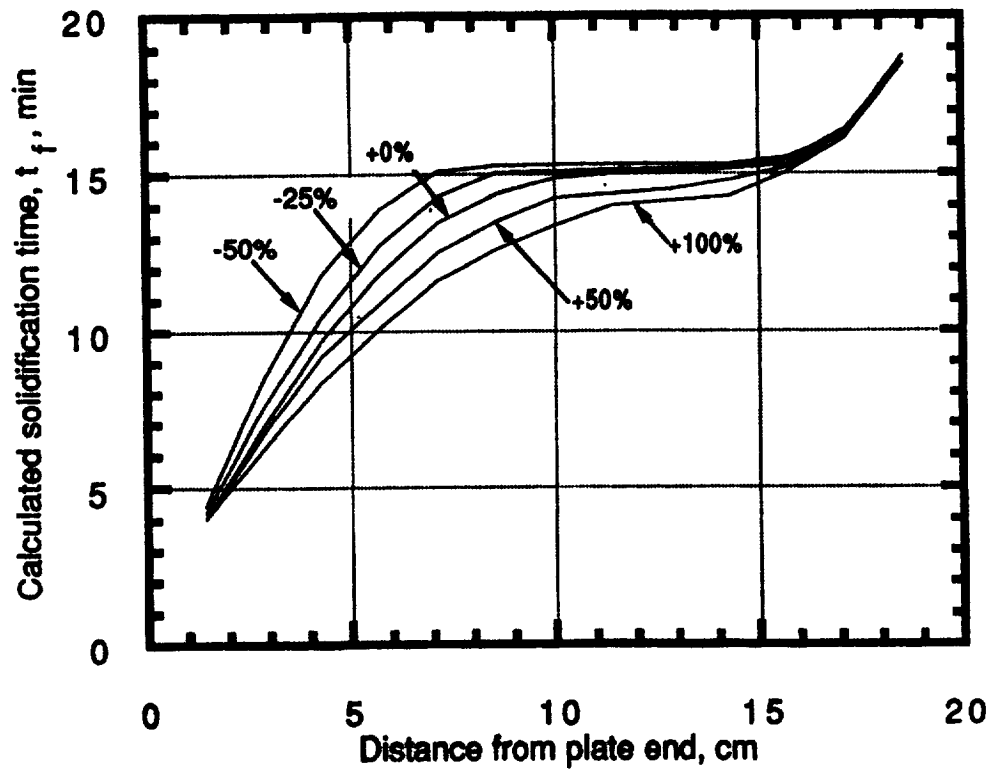




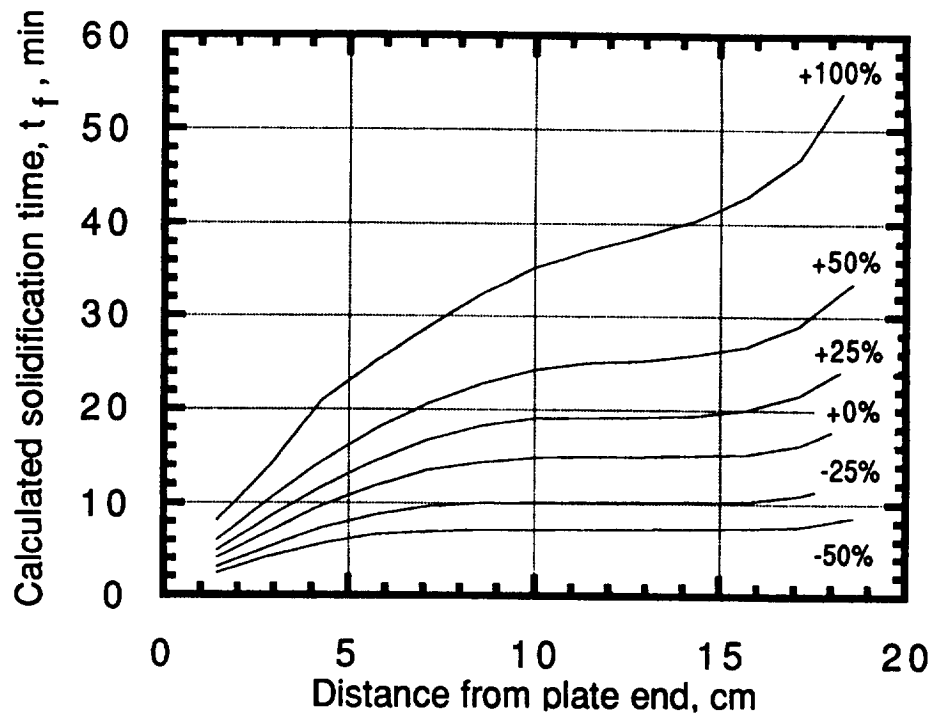
Effects of Uncertainty in Specific Heat



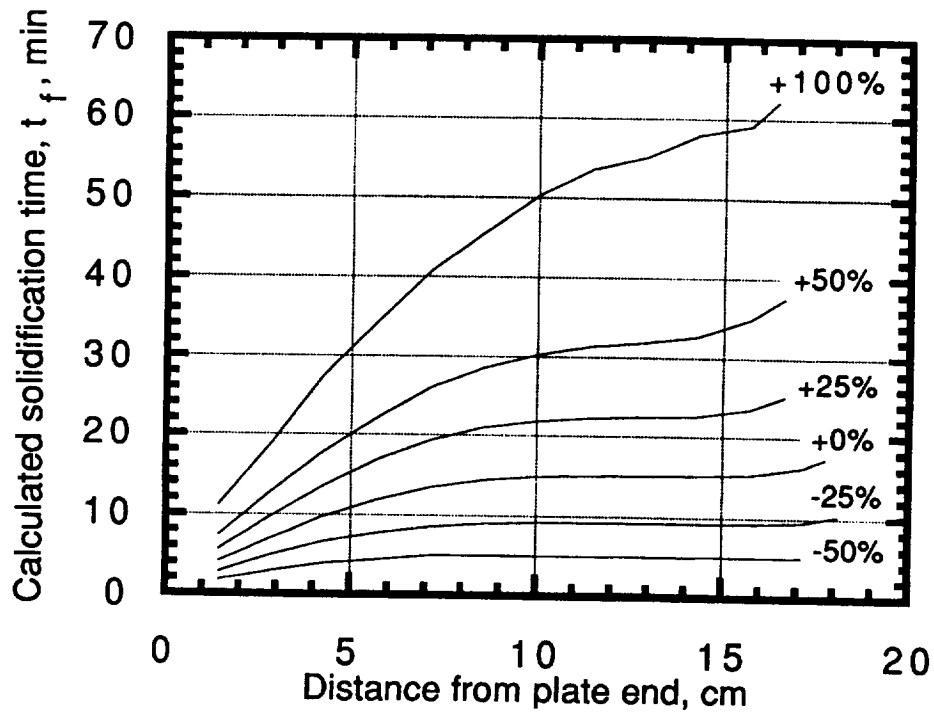
Effects of Uncertainty in Thermal Conductivity



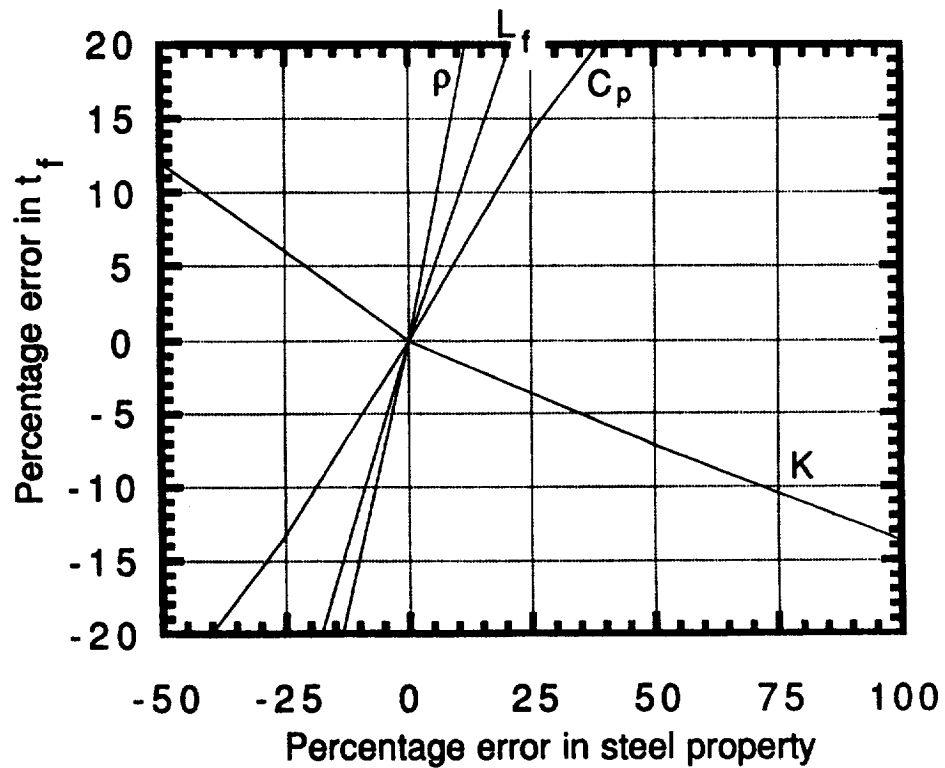
Effects of Uncertainty in Latent Heat



Effects of Uncertainty in Density



Effects of Errors In Molten Steel Properties



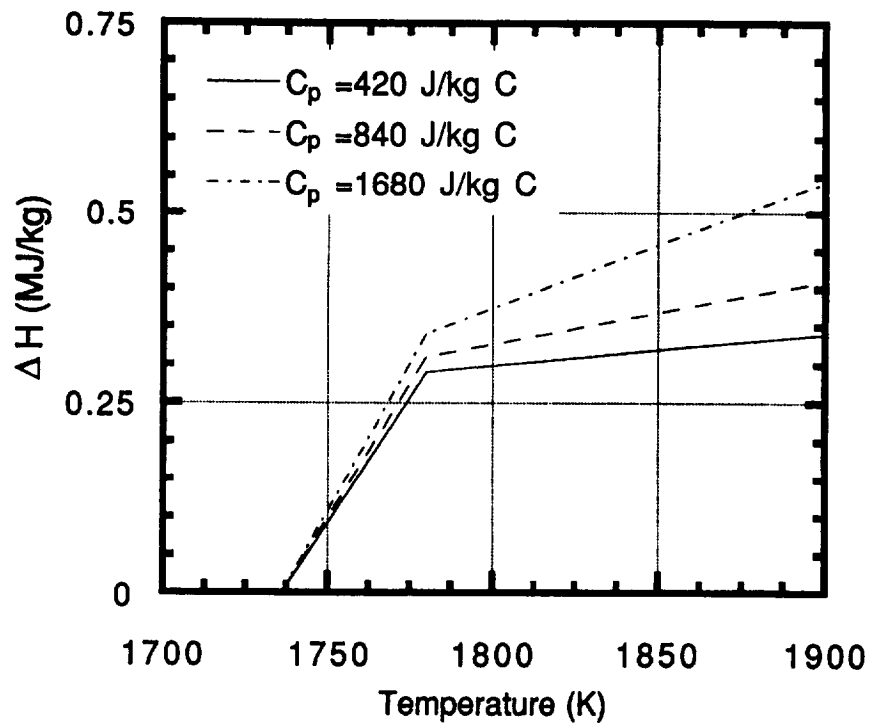
The finite element model calculates an effective specific heat from a supplied enthalpy vs. temperature curve.

$$c_p = \frac{dH/dt}{dT/dt}$$

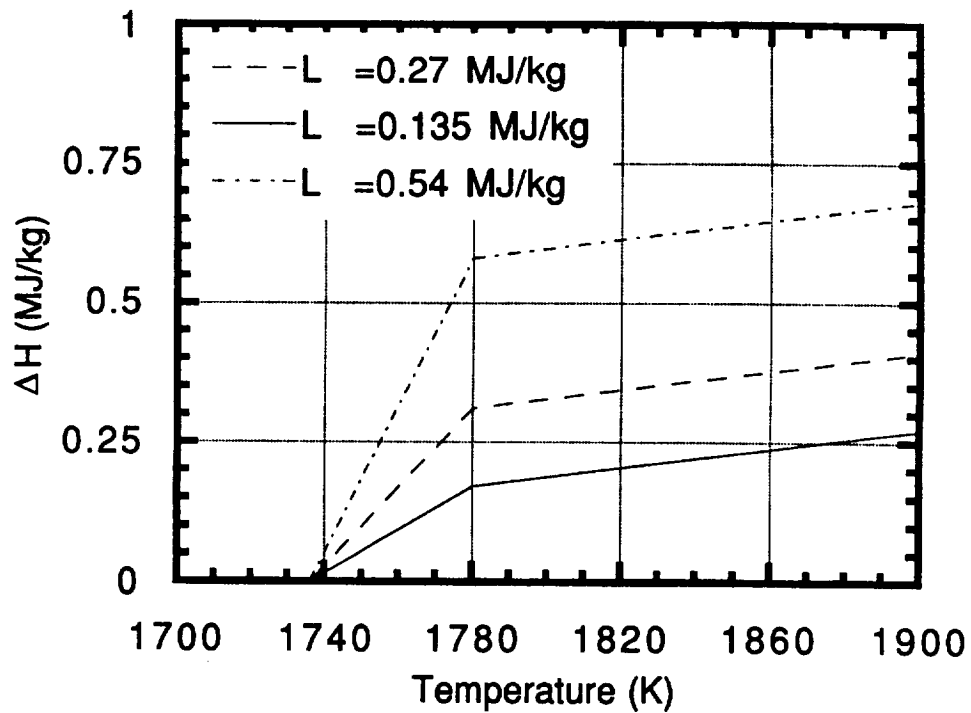
Thus c_p is determined at each integration point or nodal point:

$$c_p = \frac{H(T_n) - H(T_{n-1})}{T_n - T_{n-1}}$$

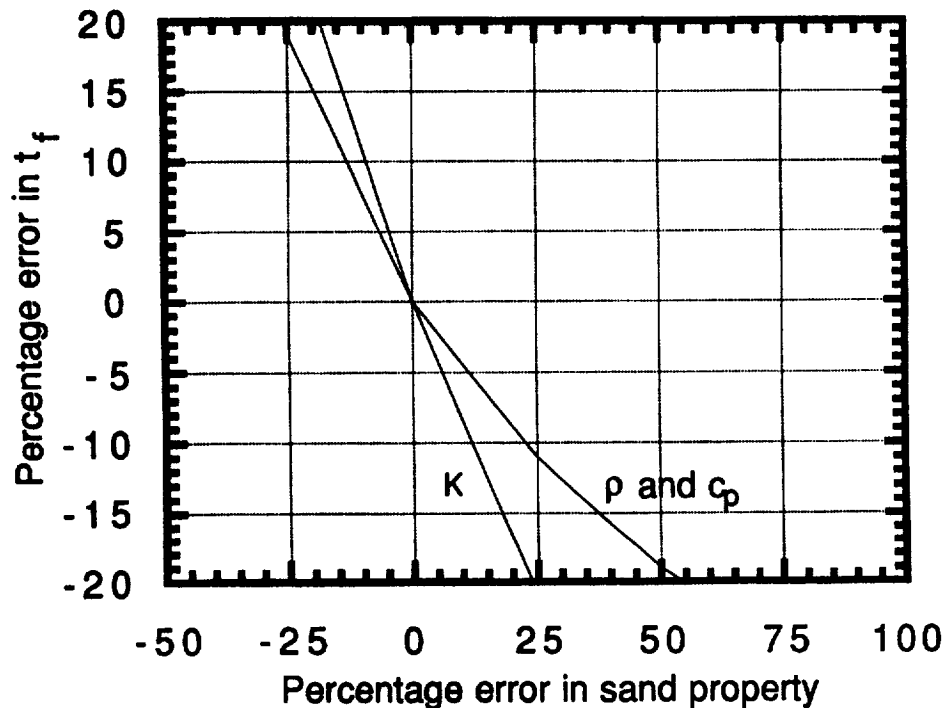
Change in Enthalpy with Different C_p 's



Change in Enthalpy with Different L_f 's



Effects of Errors in Sand Properties



Conclusions

1. The effects of uncertainties in input data can be quickly assessed by a straightforward (but computer intensive) approach.
2. The calculated cooling rate of the casting model is affected by uncertainties in the thermophysical data in the following order of influence:
 1. density
 2. latent heat
 3. thermal conductivity (sand)
 4. specific heat
 5. density and specific heat (sand)
 6. thermal conductivity
3. Similar analyses will be useful to benchmark the importance of properties in fluid flow analyses.